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The hydrated Li^+–adenine–thymine complex by IRMPD spectroscopy in the N–H/O–H stretching region

Elizabeth A.L. Gillis, Travis D. Fridgen

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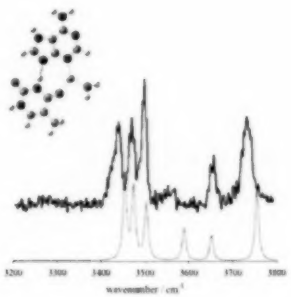
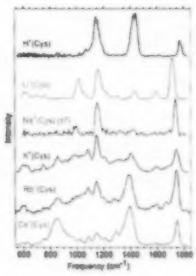


9–17

Infrared multiple photon dissociation spectroscopy of cationized cysteine: Effects of metal cation size on gas-phase conformation

Murat Citir, Elana M.S. Stennett, Jos Oomens, Jeffrey D. Steill, M.T. Rodgers, P.B. Armentrout

The gas-phase structures of M^+(Cys), where $M^+ = Li^+$, Na^+, K^+, Rb^+, Cs^+, and H^+, are examined by infrared multiple photon dissociation (IRMPD) action spectroscopy in conjunction with quantum chemical calculations.



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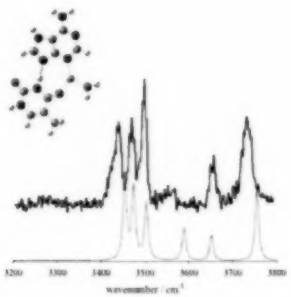

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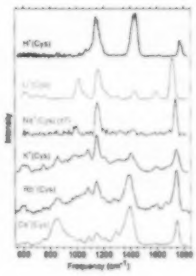

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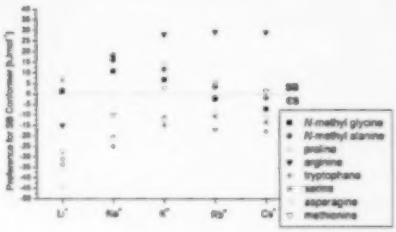
18–27

IR spectroscopy of cationized aliphatic amino acids: Stability of charge-solvated structure increases with metal cation size

Miriam K. Drayß, P.B. Armentrout, Jos Oomens, Mathias Schäfer

Stability trend of charge-solvated versus salt-bridge structures in alkali metal cationization is reversed for aliphatic versus functionalized amino acids as shown by IRMPD-spectroscopy and computational modeling.

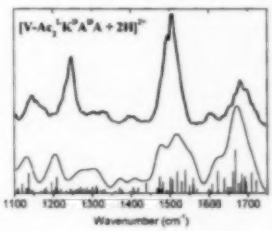


28–35

Combining ion mobility mass spectrometry and infrared multiphoton dissociation spectroscopy to probe the structure of gas-phase vancomycin–$Ac_2{}^LK^DA^DA$ non-covalent complex

Jean Christophe Poully, Frédéric Lecomte, Nicolas Nieuwjaer, Bruno Manil, Jean Pierre Schermann, Charles Desfrançois, Gilles Grégoire, Renaud Ballivian, Fabien Chirot, Jérôme Lemoine, Florent Calvo, Rodolphe Antoine, Philippe Dugourd

The structure of doubly protonated vancomycin antibiotics with its cell-wall precursor analogue $Ac_2{}^LK^DA^DA$ has been investigated in the gas phase through a combined laser spectroscopy, ion mobility and theoretical modeling approach.

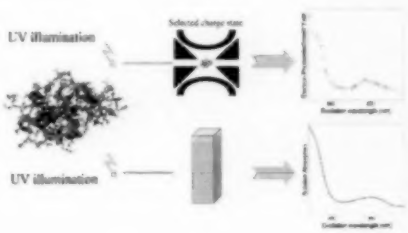


36–40

UV spectroscopy of entire proteins in the gas phase

B. Bellina, I. Compagnon, L. Joly, F. Albrieux, A.R. Allouche, F. Bertorelle, J. Lemoine, R. Antoine, Ph. Dugourd

Electron photodetachment yield measurements: an action spectroscopy for large biomolecular ions in the gas phase.

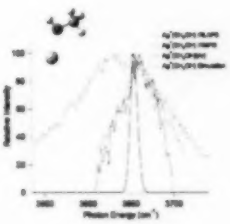


41–45

Comparison of IRMPD, Ar-tagging and IRLAPS for vibrational spectroscopy of $Ag^+(CH_3OH)$

Gokhan Altinay, Ricardo B. Metz

Three techniques – IRMPD, argon-tagging, and infrared laser-assisted photodissociation spectroscopy (IRLAPS) – are used to measure the vibrational spectra of $Ag^+(CH_3OH)$ produced under identical conditions.

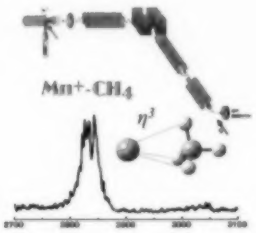


46–54

Infrared spectra and density functional theory calculations for Mn^+–$(CH_4)_n$ (n = 1–6) clusters

Viktoras Dryza, Evan J. Bieske

Infrared spectra and accompanying DFT calculations for the $Mn(CH_4)_n^+$ (n = 1–6) clusters suggest that they consist of intact methane molecules attached to a Mn^+ cation core in its ^7S ($4s^13d^5$) ground electronic state.

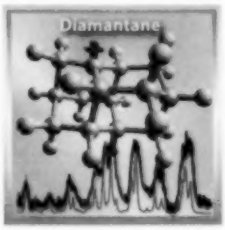


55–62

Infrared spectra and structures of diamantyl and triamantyl carbocations

Olivier Pirali, Héctor Alvaro Galué, Jeremy E. Dahl, Robert M.K. Carlson, Jos Oomens

The gas-phase IR spectra of the diamantyl and triamantyl carbocations are presented and discussed in the context of their astro-chemical relevance.

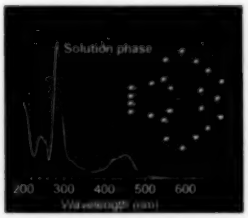


63–66

Absorption spectrum of isolated tris(2,2′-bipyridine)ruthenium(II) dications *in vacuo*

Maj-Britt Suhr Kirketerp, Steen Brøndsted Nielsen

The gas-phase absorption spectrum of tris(2,2′-bipyridine)ruthenium(II) dications has been measured and is compared to that obtained in solution.

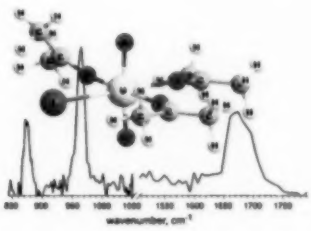


67–75

Vibrational spectra of discrete UO_2^{2+} halide complexes in the gas phase

Gary S. Groenewold, Michael J. van Stipdonk, Jos Oomens, Wibe A. de Jong, Garold L. Gresham, Michael E. McIlwain

Infrared multiple photon dissociation spectroscopy and DFT are used to investigate coordination complexes $[UO_2(X)(acetone)_3]^+$ and $[UO_2X_3]^-$, where X = halide.

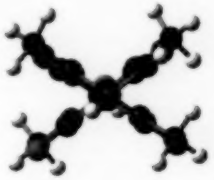


76–84

The sodium cation-bound dimer of theophylline: IRMPD spectroscopy of a highly symmetric electrostatically bound species

Richard A. Marta, Ronghu Wu, Kris R. Eldridge, Jonathan K. Martens, Terry B. McMahon

Infrared multiphoton dissociation spectroscopy and electronic structure calculations have been used to characterize the structure of a symmetric and electrostatically bound sodiated dimer of theophylline.

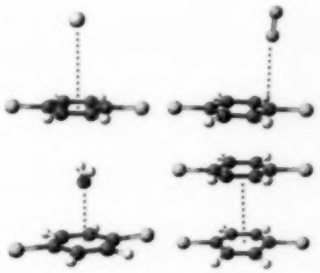


85–95

Infrared and electronic spectroscopy of p-$C_6H_4Cl_2^+$–L_n clusters with L = Ar, N_2, H_2O, and p-$C_6H_4Cl_2$

Shamik Chakraborty, Alexander Patzer, Anita Lagutschenkov, Judith Langer, Otto Dopfer

The geometric and electronic structure of the para-dichlorobenzene cation (pDCB$^+$) and its clusters with Ar, N_2, H_2O, and pDCB were characterized by vibrational and electronic spectroscopy.

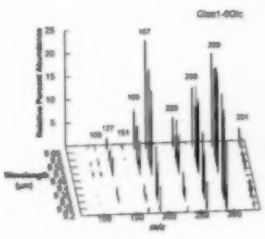


96–101

Differentiation of glucose-containing disaccharides by infrared multiple photon dissociation with a tunable CO_2 laser and Fourier transform ion cyclotron resonance mass spectrometry

Sarah E. Stefan, John R. Eyler

Wavelength-dependent fragmentation patterns of lithiated, glucose-containing disaccharides, produced with a tunable CO_2 laser, can be used to distinguish both linkage position and anomeric configurations of the disaccharides.



102–106

Infrared spectroscopic characterization of the oxidative dehydrogenation of propane by $V_4O_{10}^+$

Torsten Wende, Jens Döbler, Ling Jiang, Pieterjan Claes, Ewald Janssens, Peter Lievens, Gerard Meijer, Knut R. Asmis, Joachim Sauer

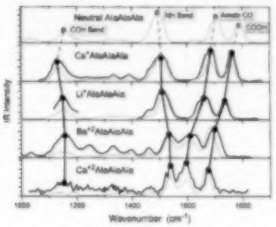
The gas phase reaction of $V_4O_{10}^+$ with propane is studied by infrared photodissociation spectroscopy combined with density functional calculations.

107–115

Conformations and vibrational spectroscopy of metal-ion/polylalanine complexes

Robert C. Dunbar, Jeffrey D. Steill, Jos Oomens

Metal-ion complexes of dialanine and dialanine are reported for alkali and alkaline earth ions. Metal/ligand interaction effects on conformations and normal mode frequencies are determined using IRMPD spectroscopy combined with computation.

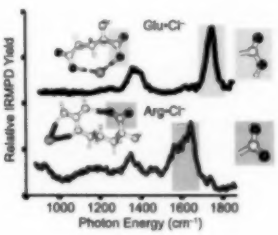


116–123

Effects of anions on the zwitterion stability of Glu, His and Arg investigated by IRMPD spectroscopy and theory

Jeremy T. O'Brien, James S. Prell, Giel Berden, Jos Oomens, Evan R. Williams

The effects of halide ions on the zwitterion stability of Glu, His and Arg were investigated using IRMPD spectroscopy and hybrid density functional theory.

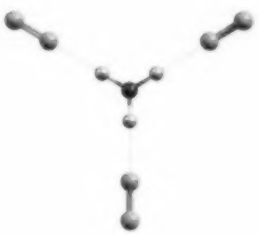


124–130

Proton sharing in hydronium–nitrogen clusters probed with infrared spectroscopy

B. Bandyopadhyay, T.C. Cheng, M.A. Duncan

Hydronium nitrogen cluster ions are studied in the free-OH and hydrogen bonding regions with infrared photodissociation spectroscopy.

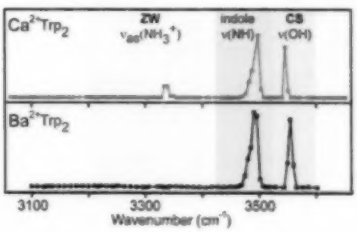


131–138

Vibrational signatures of zwitterionic and charge-solvated structures for alkaline earth-tryptophan dimer complexes in the gas phase

Warren K. Mino Jr., Jan Szczepanski, W. Lee Pearson, David H. Powell, Robert C. Dunbar, John R. Eyler, Nick C. Polfer

Diagnostic vibrations for alkaline earth-tryptophan dimers, $M^{2+}Trp_2$, confirm mixed CS/ZW (charge solvation/Zwitterion)complexes for Mg and Ca, as opposed to CS/CS for Sr and Ba.

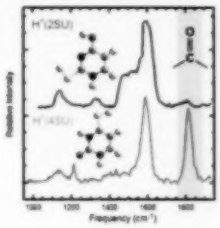


139–151

Infrared multiple photon dissociation action spectroscopy of protonated uracil and thiouracils: Effects of thioketo-substitution on gas-phase conformation

Y.-w. Nei, T.E. Akinyemi, J.D. Steill, J. Oomens, M.T. Rodgers

The gas-phase structures of protonated complexes of uracil and five thiouracils are examined via IRMPD action spectroscopy and theoretical calculations. Present results indicate that protonation stabilizes minor tautomers of these nucleobases.

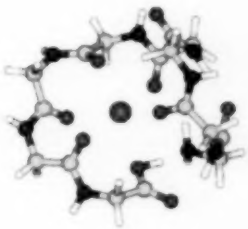


152–161

Assessment of density functionals for predicting the infrared spectrum of sodiated octa-glycine

David Semrouni, Carine Clavaguéra, Jean-Pierre Dognon, Gilles Ohanessian

Various density functionals were evaluated to reproduce the structure and the infrared spectrum of the octa-glycine complexed to the sodium ion.

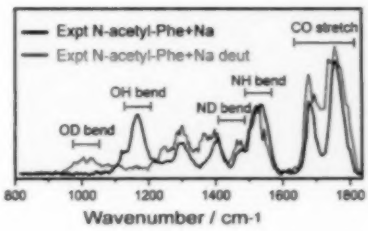


162–169

Hydrogen/deuterium exchange of phenylalanine analogs studied with infrared multiple photon dissociation

Cesar S. Contreras, Nicolas C. Polfer, Alfred C. Chung, Jos Oomens, John R. Eyler

► IRMPD spectra are reported for three phenylalanine analogs following both gas-phase and solution-phase H/D exchange reactions. ► Gas-phase exchange results exclusively in replacement of the carboxylic acid H with D. ► Solution-phase exchange leads to replacement of carboxylic acid, amide, and amine hydrogens.



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